Theodore L. Fobe

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Education

University of Colorado, Boulder, CO
College of Engineering & Applied Science
PhD Student, Chemical Engineering, May 2022
PhD Advisor, Michael R. Shirts
GPA: **3.94**

University of Maryland, College Park, MD
A. James Clark School of Engineering
BS, Chemical Engineering, May 2018, *Cum Laude*
College of Computer, Mathematical and Natural Sciences
BS, Biochemistry, May 2018
GPA: **3.90** (Cumulative), **3.93** (Chemical Engineering), **3.85** (Biochemistry)

Honors and Society Memberships

Tau Beta Pi, National Engineering Honor Society (September 2015 – May 2018)
Omega Chi Epsilon, National Honor Society for Chemical Engineering (September 2015 – May 2018)
University of Maryland, College Park, Scholars Program, Science and Global Change (August 2014 – May 2016)
Philip Merrill Presidential Scholarship (2014-15)
Donald Lee Huston Memorial Scholarship (2016-2017)
Mildred and Clark Steyer Scholarship (2016-2017)
Walter Schymik Undergraduate Research Scholarship (2017-2018)
G. Forrest Woods Memorial Scholarship (2017-2018)
GAANN Soft Materials Fellowship (2019-2020, 2020-2021)

Work Experience

Shirts Research Group *Graduate Student* (August 2018 – Current)
Investigating secondary structure in atomistic and coarse-grained models of non-biological heteropolymers
Setup and performed molecular simulations combined with several enhanced sampling methods
Developed software packages following coding best practices

NIST Boulder Laboratories *Summer Undergraduate Research Fellowship* (May 2017–August 2018, May 2018 – August 2019)
Researched structural bioinformatics involving disulfide bonds in proteins
Helped develop Cys.sqlite a comprehensive cysteine/disulfide bond database
Performed elastic network model simulations of proteins to quantify disulfide bond effects on protein structure and dynamics

Laboratory of Thermodynamic and Molecular Modeling *Student Researcher* (May 2015 – May 2018)
Researched pore formations in lipid bilayers containing ceramides for transdermal drug delivery
Performed NAMD simulations of varying ceramide concentrations under various conditions
Developed and edited NAMD and CHARMM scripts for manipulating and analyzing simulations

University of Maryland, College Park *Undergraduate Teaching Assistant* (August 2017 – May 2018)
Assisted teaching courses in the Chemical & Biomolecular Engineering Department, the Chemistry and Biochemistry Department and the Physics Department
Was responsible for grading homework, exams and holding office hours.

Leadership Experiences

Graduate Leadership Committee *Social Chair* (May 2021-Current) *Outreach Chair* (Jan 2020-April 2021)
Planned outreach and social events for graduate students in the Chemical and Biological Engineering Department
Worked closely with department chairs and building services to reserve rooms and execute events
Managed the budget for social events

NIST SURF *Committee Chair* (May 2018 – August 2018)
Planned and coordinated the end of summer research colloquium for both SHIP/SURF programs
Worked closely with NIST SURF directors to organize a technical scientific program

Omega Chi Epsilon Research Day *Committee Head* (October 2015-May 2018)
Organized an undergraduate research presentation event for Omega Chi Epsilon for 3 consecutive years
Lead bi-weekly meetings with a team of students to prepare for the poster competition

Tau Beta Pi *Community Service Chair* (May 2016 -May 2017)
Planned several community service and educational outreach events for Tau Beta Pi's MD Beta Chapter
Worked with non-profit organizations, such as A Wider Circle and Martha's Table to plan service events

Teaching Experiences

University of Colorado Boulder (2018 - Present):

Fall 2021	Teaching Assistant/Lecturer, CHEN 5370: Intermediate Chemical Engineering Thermodynamics
Spring 2019	Teaching Assistant, CHEN 4521: Physical Chemistry for Engineers

University of Maryland, College Park (2014-2018):

Spring 2018	Teaching Assistant/Instructor, CHEM242: Organic Chemistry Laboratory II
Fall 2017	Teaching Assistant/Instructor, CHEM242: Organic Chemistry Laboratory II
Fall 2017	Teaching Assistant, CHBE440: Chemical Kinetics and Reactor Design
Spring 2017	Teaching Assistant, CHBE302: Chemical and Biomolecular Engineering Thermodynamics II
Fall 2017	Teaching Assistant, CHBE250: Chemical and Biomolecular Engineering Thermodynamics II
Spring 2016	Teaching Assistant, PHYS270: Electrodynamics, Light, Relativity and Modern Physics

Mentorship Experiences

ChBE Peer Mentor (2019-2020, 2021-2022, 2022-2023)

- Mentored three first year students in the ChBE program to help their transition to graduate school
- Gave advice on mentor selection, research, graduate courses and work life balance in graduate school
- Attended graduate school mentorship events such as the welcome hike and picnic and advisor speed dating

Undergraduate Research Mentor (2019-2020, May 2020-August 2020)

- Worked closely with two undergraduate research assistants in the Shirts group
- Developed a summer research plan a visiting undergraduate researcher
- Lead weekly meetings with students to advise on research direction and ensure they were making progress

Technical Skills

Python, C++, Rosetta/PyRosetta, GROMACS, Bash, Perl, MATLAB, CHARMM, NAMD, R, ASPEN Plus, MATHCAD, Inventor (CAD) and Microsoft Office Suites

Github Contributions

Heteropolymer Simulations:
A repository for performing and analyzing simulations of non-biological heteropolymers. This repository contains several GROMACS simulation parameter files for standard MD simulations, replica exchange MD simulations and metadynamics simulations. I primarily developed this repository.
www.github.com/shirtsgroup/heteropolymer_simulations

CG PyRosetta:
A repository which implements custom CG potentials in the python-wrapped macromolecule design software, PyRosetta.. This repository contains several CG foldamer residue parameter files which were used to generate results for the JCTC paper titled "*Folding Coarse-Grained Oligomer Models with PyRosetta*". I primarily developed this repository.
www.github.com/shirtsgroup/cg_pyrosetta

Rosetta:
A repository that contains the source code for Rosetta, a popular macromolecule design software. I contributed a PR that added functionality to load new molecular mechanics score function parameters from the command line.
www.github.com/RosettaCommons/main

Boltzmann Generators:
A repository that implements Boltzmann generators for a variety of test systems. I helped develop this repository for a final project in a simulation methods class. I implemented two test systems and applied Boltzmann generators to the output of their simulations.
www.github.com/tlfobe/boltzmann_generators

Cys.SQLite:
A repository that holds code to build a database of cysteine bonds from the most recent version of the PDB. I helped implement the SQL schema during a NIST SURF. I contributed code to generate 2D phi/psi histograms and helped develop the original schema used in the database.
www.github.com/usnistgov/Cys.sqlite

Publications

T. L. Fobe, C. C. Walker, G. A. Meek, M. R. Shirts, **"Folding Coarse-Grained Oligomer Models with PyRosetta,"** *J. Chem. Theory Comput.,* Sept. 2022.

C. C. Walker, **T. L. Fobe**, M. R. Shirts, **"How Cooperatively Folding Are Homopolymer Molecular Knots?,"** *Macromolecules, Oct. 2021*

C. C. Walker, G. A. Meek, **T. L. Fobe**, M. R. Shirts, **"Using a Coarse-Grained Modeling Framework to Identify Oligomeric Motifs with Tunable Secondary Structure,"** *J. Chem. Theory Comput.,* Aug. 2021.

A. F. Kleman, D. L. Dufek, **T. L. Fobe**, D. R. McCaslin, B. P. Cary, M. R. Shirts, S. H. Gellman, **"Potential Foldamers Based on an *ortho*-Terphenyl Amino Acid,"** Org. Lett., June 2021.

T. L. Fobe, A. Kazakov, and D. Riccardi, **"Cys.sqlite: A Structured-Information Approach to the Comprehensive Analysis of Cysteine Disulfide Bonds in the Protein Databank,"** *J. Chem. Inf. Model.*, Jan. 2019.

A. Mengis, **T. Fobe**, R.D. Sochol, *et al,* **"Nano 3D Printing-Enabled Micropost Array Gradients,"** Proceedings of the 30th IEEE International Conference on Micro Electro Mechanical Systems (IEEE MEMS 2017), Las Vegas, NV, USA.

Conference Presentations

T. L. Fobe, C. C. Walker, M. R. Shirts, **"Investigating Foldamer Secondary Structure in Coarse- and Fine-grained Models,"** Proceedings of the 2023 ACS Spring Meeting, Indianapolis, IN, USA (talk).

T. L. Fobe, C. C. Walker, M. R. Shirts, **"Investigating Novel Terphenyl Oligomer Secondary Structure using Enhanced Sampling Methods,"** RJ8 Computational Design and Modeling of Biomolecules, 2023, Banff, AB, CA (poster).

T. L. Fobe, C. C. Walker, M. R. Shirts, **"Folding Coarse-Grained Foldamer Models with PyRosetta,"** Proceedings of the 2022 ACS Fall Meeting, Chicago, IL, USA (talk).

T. L. Fobe, C. C. Walker, M. R. Shirts, **"Folding Coarse-Grained Oligomer Models With PyRosetta,"** Summer RosettaCon 2022, Leavenworth, WA, USA (poster).

T. L. Fobe, C. C. Walker, M. R. Shirts, **"Exploring Non-Biological Foldamer Secondary Structure Using Tuneable Coarse-Grained Models,"** Proceedings of the 2021 AIChE Annual Meeting (talk).

T. L. Fobe, C. C. Walker, G. A. Meek, M. R. Shirts, **"Exploring Coarse-Grained Foldamer Secondary Structure using PyRosetta,"** Summer RosettaCon 2021 (virtual poster).

T. L. Fobe, C. C. Walker, G. A. Meek, M. R. Shirts, **"CG PyRosetta: A Coarse-Grained Configuration Search Tool for General Foldamer Secondary Structure,"** Proceedings of the 2020 Virtual AIChE Annual Meeting (virtual poster).

T. L. Fobe, G. A. Meek, M. R. Shirts, **"CG PyRosetta: A Coarse-Grained Configuration Search Tool for General Foldamer Secondary Structure,"** Winter RosettaCon 2020, New York, NY, USA (poster).

T. Fobe, D. Riccardi, **"Structural and energetic analysis of disulfide bonds in the protein data bank,"** Proceedings of the 2017 AIChE Annual Meeting, Minneapolis, MN, USA (poster).